

## New and Practical Formulation for Overlaps of Bogoliubov Vacua

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In this Letter, we present a new expression for the overlaps of wave functions in Hartree-Fock-Bogoliubov based theories. Starting from the Pfaffian formula by Bertsch *et al.* [1], an exact and computationally stable formula for overlaps is derived. We illustrate the convenience of this new formulation with a numerical application in the context of the particle-number projection method. This new formula allows for substantially increased precision and versatility in chemical, atomic, and nuclear physics applications, particularly for methods dealing with superfluidity, symmetry restoration, and uses of nonorthogonal many-body basis states.

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*Introduction.*—A very successful approach in the context of many-body theory is to incorporate correlation effects through symmetry breaking followed by restoration of symmetries [2]. The intuitive picture gained from the symmetry-broken solutions has provided much insight into the symmetry and beauty of nature. For instance, many nuclei can be described as intrinsically deformed where both axial and reflection symmetry are broken [3]. Moreover, combining shape degrees of freedom with angular momentum orientation, additional symmetries arise that can also be broken with spectacular manifestations in nuclear spectra [4]. For each broken symmetry new collective modes emerge, which complete a picture of nuclear structure and nuclear spectra with an increasing precision. As starting points, mean-field theories play a large role because of their ability to find approximate solutions to the many-body Schrödinger equation at a relatively low computational cost [5]. A typical example is the Hartree-Fock-Bogoliubov (HFB) method where the wave function solution is written as a product of independent quasiparticles. Nuclear physics applications of HFB coupled with symmetry-restoration methods have allowed us to accurately describe a vast swath of nuclear properties such as binding energies, mean-square radii, deformation, and spectra. Under certain circumstances, such as for instance in the case of shape coexistence, it becomes necessary to include additional correlations between the quasiparticles. Correlations beyond the mean field can be included, for example, using the framework of the generating coordinate method (GCM) [5–11] where

the wave function is written as a linear combination of different nonorthogonal mean-field configurations. In practice, the solution of GCM equations and the application of symmetry-restoration methods require the precise computation of overlap functions. The modulus of the overlap between two HFB vacua can be computed with the Onishi formula [12] thus leaving ambiguity on its sign. Several studies have subsequently been dedicated to compute the overlap using various methods [13–23]. In [24], Robledo derived an expression for the overlap in terms of a Pfaffian (pf). In a later publication [1], Bertsch and Robledo extended the Pfaffian formulation to overlaps between odd-*A* systems and overlaps for operators involved in symmetry-restoration methods. Let us consider two HFB vacua  $|\Phi\rangle$  and  $|\Phi'\rangle$  with even number parity (for an even-*A* nucleus) and the associated overlap  $\mathcal{O} \equiv \langle \Phi | \Phi' \rangle$ . The formula by Bertsch and Robledo [1] gives  $\mathcal{O}$  as

$$\mathcal{O} = (-1)^{N/2} \frac{(\det C)^* \det C'}{\prod_{i,i'} v_i v_{i'}} \text{pf} \begin{pmatrix} V^T U & V^T V'^* \\ -V'^{\dagger} V & U'^{\dagger} V'^* \end{pmatrix}, \quad (1)$$

where  $N$  is the (even) number of single-particle basis states and  $U, V$  ( $U', V'$ ) are matrices of the Bogoliubov transformation associated with  $|\Phi\rangle$  ( $|\Phi'\rangle$ ) [5]. Using the Bloch-Messiah decomposition [25], one can write  $U = D\bar{U}C$  and  $V = D^*\bar{V}C$  where  $D$  and  $C$  are both unitary matrices and  $D$  defines the so-called canonical basis associated with  $|\Phi\rangle$ .  $\bar{U}$  and  $\bar{V}$  can be chosen as diagonal and skew-symmetric, respectively. The matrix  $\bar{V}$  is written in terms of  $N/2$  blocks of dimension  $2 \times 2$  with elements  $(v_i, -v_i)$  where  $v_i^2$  is the occupation probability of the canonical basis state  $i$  (the matrix elements  $u_i$  of  $\bar{U}$  are such that  $u_i^2 + v_i^2 = 1$ ). We adopt the usual phase convention  $u_i > 0$  and  $v_i > 0$  [5]. For  $v_i = 1$ , the level  $i$  is fully occupied whereas it is empty for  $v_i = 0$ .  $v_i$  and  $C'$  in

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(1) are obtained by the Bloch Messiah decomposition of  $(U', V')$ . In practice, due to the tiny values of  $v_i, v'_i$  for the least occupied levels, the computation of the overlap (1) can become unstable. Indeed, in this context, both the denominator  $\prod_{i,i'} v_i v'_i$  and the Pfaffian in the numerator of Eq. (1) have small values that can become out of the scope of the double-precision data type. A potential solution to this issue could be to discard levels for which  $v_i, v'_i \sim 0$  in the computation of the overlap. But in practice, it can become difficult to check the reliability of such an approach. Indeed, one would need to check that the omitted levels have a negligible contribution in the value of the overlap and this would be done by increasing the number of levels considered. Eventually one might again run into instability of the numerical computation. It is especially important to obtain precise values of overlaps in the context of GCM where the basis states are not orthogonal and requires the solution of a generalized eigenvalue problem in the overcomplete basis. Other solutions to this issue have been proposed in [26] where small values of  $v_i$  are replaced by an *ad hoc* tiny numerical parameter  $\epsilon$ . However, it would be advantageous and more convenient for systematic calculations to be able to bypass the introduction of such a parameter. It should be mentioned that similar issues with multiplications of large and small terms were also discussed in [13] where, using a different formulation of the overlap, difficulties arise instead for  $u_i, u'_i \sim 0$ . This formulation was further generalized in [22,27] where tailored algorithmic procedures were introduced to allow for inclusion of states having exactly  $u_i, u'_i = 0$ . Nevertheless, in practice the presence of states with very small but nonzero values of  $u_i, u'_i = 0$  still requires the introduction of a cutoff.

In this Letter, we present a new and practical formulation of the overlap [see Eq. (10) in the case of an even- $A$  system and Eq. (12) for an odd- $A$  system] which allows for a precise and stable computation and is also amenable to controllable truncations. This Letter is organized as follows. We first show the main steps involved in the derivation of the formula for the overlap between two HFB vacua for an even- $A$  system and then show the expression for the overlap in the case of an odd- $A$  system. We then illustrate the numerical stability offered by this formulation by computing, as a function of the number of canonical basis states included, the matrix element of the particle-number projection operator.

We start the derivations from Eq. (1). First, we want to point out that this equation cannot be used directly when including empty levels since in that case, the expression

involves products of zero and infinity. The equation is, however, generally valid if one assumes a tiny occupation  $\epsilon$  for the empty levels. In our final expression Eqs. (10) and (12), these factors cancel out analytically and one may safely evaluate the expression in the limit  $\epsilon \rightarrow 0$ .

We denote  $M$  the matrix argument of the Pfaffian in Eq. (1). Using the Bloch-Messiah decomposition for  $U, V$  and  $U', V'$  we obtain

$$\begin{aligned} M &= \begin{pmatrix} -C^T \bar{V} \bar{U} C & -C^T \bar{V} D^\dagger D' \bar{V}' C'^* \\ C'^\dagger \bar{V}' D'^T D^* \bar{V} C & C'^\dagger \bar{U}' \bar{V}' C'^* \end{pmatrix} \\ &= \begin{pmatrix} C^T & 0 \\ 0 & C'^\dagger \end{pmatrix} \begin{pmatrix} -\bar{V} \bar{U} & -\bar{V} D^\dagger D' \bar{V}' \\ \bar{V}' D'^T D^* \bar{V} & \bar{U}' \bar{V}' \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C'^* \end{pmatrix}. \end{aligned} \quad (2)$$

From Eq. (2) and the relation

$$\text{pf}(ABA^T) = \det(A)\text{pf}(B), \quad (3)$$

we can write

$$\text{pf}(M) = \det C \det C'^\dagger \text{pf} \begin{pmatrix} -\bar{V} \bar{U} & -\bar{V} D^\dagger D' \bar{V}' \\ \bar{V}' D'^T D^* \bar{V} & \bar{U}' \bar{V}' \end{pmatrix}. \quad (4)$$

In order to avoid the numerical instability that arises in the computation of the overlap directly from Eq. (1) we factorize the norms of the HFB vacua out of  $\text{pf}(M)$ . This is achieved in the following steps by first writing the matrix argument of the Pfaffian on the right-hand side of Eq. (4) as

$$\begin{pmatrix} \bar{V} & 0 \\ 0 & \bar{V}' \end{pmatrix} \begin{pmatrix} \bar{U} \bar{V}^{-1} & D^\dagger D' \\ -D'^T D^* & -\bar{V}'^{-1} \bar{U}' \end{pmatrix} \begin{pmatrix} -\bar{V} & 0 \\ 0 & -\bar{V}' \end{pmatrix}. \quad (5)$$

Introducing the diagonal matrix

$$\Lambda = \begin{pmatrix} \sqrt{v_0} & & & & \\ & \sqrt{v_0} & & & \\ & & \sqrt{v_1} & & \\ & & & \ddots & \\ & & & & \sqrt{v_{N/2-1}} \end{pmatrix} \quad (6)$$

and a similar matrix  $\Lambda'$  with the occupation number  $v'_i$ , we can rewrite (5) as

$$\begin{pmatrix} \bar{V} \Lambda^{-1} & 0 \\ 0 & \bar{V}' \Lambda'^{-1} \end{pmatrix} \begin{pmatrix} \Lambda \bar{U} \bar{V}^{-1} \Lambda & \Lambda D^\dagger D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & -\Lambda' \bar{V}'^{-1} \bar{U}' \Lambda' \end{pmatrix} \begin{pmatrix} -\Lambda^{-1} \bar{V} & 0 \\ 0 & -\Lambda'^{-1} \bar{V}' \end{pmatrix}. \quad (7)$$

From the expression above, we can now write Eq. (4) as

$$\text{pf}(M) = \det C \det C'^{\dagger} \text{pf} \left[ \begin{pmatrix} \bar{V}\Lambda^{-1} & 0 \\ 0 & \bar{V}'\Lambda'^{-1} \end{pmatrix} \begin{pmatrix} \Lambda\bar{U}\bar{V}^{-1}\Lambda & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & -\Lambda' \bar{V}'^{-1} \bar{U}' \Lambda' \end{pmatrix} \begin{pmatrix} -\Lambda^{-1} \bar{V} & 0 \\ 0 & -\Lambda'^{-1} \bar{V}' \end{pmatrix} \right] \quad (8)$$

$$= \det C \det C'^{\dagger} \det(\bar{V}\Lambda^{-1}) \det(\bar{V}'\Lambda'^{-1}) \text{pf} \begin{pmatrix} \Lambda\bar{U}\bar{V}^{-1}\Lambda & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & -\Lambda' \bar{V}'^{-1} \bar{U}' \Lambda' \end{pmatrix}, \quad (9)$$

where Eq. (9) has been obtained from Eq. (8) using once again the relation (3). The matrix  $\bar{V}\Lambda^{-1}$  is tridiagonal and skew symmetric with matrix elements  $\sqrt{v_i}$  and  $-\sqrt{v_i}$ . As a consequence, one has  $\det(\bar{V}\Lambda^{-1}) = \prod_i v_i$  and similarly  $\det(\bar{V}'\Lambda'^{-1}) = \prod_i v'_i$ . As it becomes clear now, the *ad hoc* introduction of  $\Lambda$  and  $\Lambda'$  has allowed us to factorize the norm of the HFB vacua out of the Pfaffian in Eq. (4). Using Eq. (9) in Eq. (1), we now arrive at an expression of the overlap as

$$\begin{aligned} & (-1)^{N/2} \text{pf} \begin{pmatrix} \Lambda\bar{U}\bar{V}^{-1}\Lambda & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & -\Lambda' \bar{V}'^{-1} \bar{U}' \Lambda' \end{pmatrix} \\ &= (-1)^{N/2} \text{pf} \begin{pmatrix} -\bar{U}\sigma & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & \sigma \bar{U}' \end{pmatrix}, \quad (10) \end{aligned}$$

where  $\sigma$  is the  $N \times N$  tridiagonal skew-symmetric matrix with elements 1 and  $-1$  [28]. The expression (10) is exact and allows for a stable numerical computation of overlaps independently of how tiny the occupation number  $v_i$  might be (this includes the limit of vanishing occupations, e.g., in the case of no pairing, where occupation numbers are exactly 0 for levels with energy greater than the Fermi energy). Moreover, the formula enables us to systematically reduce the computing cost by including only levels for which the occupation number  $v_i$  ( $v'_i$ ) is greater than a given value  $\eta$  and accordingly truncating the matrix in Eq. (10). The quality of the truncation can then be checked *a posteriori* by decreasing  $\eta$  to arbitrary small values. Let us assume that for a given value of  $\eta$ ,  $n$  ( $n'$ ) canonical basis states fulfill the criteria  $v_i \geq \eta$  ( $v'_i \geq \eta$ ). In that case, the values of the overlap in this truncated space is given by [28]:

$$(-1)^{n/2} \text{pf} \begin{pmatrix} [-\bar{U}\sigma]_{n \times n} & [\Lambda D^{\dagger} D' \Lambda']_{n \times n'} \\ -[\Lambda' D'^T D^* \Lambda]_{n' \times n} & [\sigma \bar{U}']_{n' \times n'} \end{pmatrix}. \quad (11)$$

$$\mathcal{O} = (-1)^{n/2} \text{pf} \begin{pmatrix} -[\bar{U}\sigma]_{n \times n} & [\Lambda D^{\dagger} D' \Lambda']_{n \times n'} & [\Lambda D^{\dagger} \mathbf{V}^{(a)*}]_{n \times 1} & [\Lambda D^{\dagger} \mathbf{U}'^{(a')}]_{n \times 1} \\ & [\sigma \bar{U}']_{n' \times n'} & -[\Lambda' D'^T \mathbf{U}^{(a)*}]_{n' \times 1} & -[\Lambda' D'^T \mathbf{V}'^{(a')}]_{n' \times 1} \\ & & 0 & [\mathbf{U}^{(a)\dagger} \mathbf{U}'^{(a')}]_{1 \times 1} \\ & & & 0 \end{pmatrix}. \quad (16)$$

The extension for odd- $A$  systems is straightforward and the derivation goes along the same line (see [28]). Let us consider the overlap between two odd- $A$  states written as one quasiparticle creation operators acting on even-number-parity HFB vacua that is,  $\beta_a^{\dagger} |\Phi\rangle$  and  $\beta_{a'}^{\dagger} |\Phi'\rangle$ . The corresponding overlap  $\langle \Phi | \beta_a \beta_{a'}^{\dagger} | \Phi' \rangle$  is given as

$$\mathcal{O} = (-1)^{N/2} \text{pf} \begin{pmatrix} A & B \\ -B^T & C \end{pmatrix} \quad (12)$$

with matrix

$$A = \begin{pmatrix} -\bar{U}\sigma & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^T D^* \Lambda & \sigma \bar{U}' \end{pmatrix}, \quad (13)$$

related to the even part of the system,

$$B = \begin{pmatrix} \Lambda D^{\dagger} & 0 \\ 0 & -\Lambda' D'^T \end{pmatrix} \begin{pmatrix} \mathbf{V}^{(a)*} & \mathbf{U}'^{(a')} \\ \mathbf{U}^{(a)*} & \mathbf{V}'^{(a')} \end{pmatrix} \quad (14)$$

related to the connection between the even and the odd part and

$$C = \begin{pmatrix} 0 & \mathbf{U}^{(a)\dagger} \mathbf{U}'^{(a')} \\ -\mathbf{U}^{(a)\dagger} \mathbf{U}'^{(a')} & 0 \end{pmatrix} \quad (15)$$

related to the odd particles. The index  $a$  ( $a'$ ) in the equations above is used to denote the column vectors associated with the two blocked quasiparticles. As in the case of the overlap between even-number-parity vacua, the expression for the overlap in the odd case is numerically stable and allows for controllable truncations. In this context, the truncated expression for the overlap can be written as [31] (see [28]):

*Example.*—As a proof of principle, we now show results for the computation of a matrix element involved in the particle-number projection method for an even- $A$  nucleus. We denote this matrix element  $\mathcal{O}^{\text{PN}}$ :

$$\mathcal{O}^{\text{PN}} \equiv \langle \Phi | e^{-i\hat{N}\phi} | \Phi \rangle = \langle \Phi | \Phi' \rangle, \quad (17)$$

where  $e^{-i\hat{N}\phi}$  is the gauge rotational operator for the particle-number projection,  $\hat{N}$  the particle-number operator, and  $\phi$  the gauge angle. We focus on projecting the number of neutrons and generate the occupation numbers with a HFB calculation of  $^{192}\text{Pb}$  using a basis of 17 major oscillator shells, the SLY4 functional [32], and a separable Gaussian pairing interaction [33]. We rewrite  $\mathcal{O}^{\text{PN}}$  as the overlap between the vacuum  $|\Phi\rangle$  and a rotated vacuum  $|\Phi'\rangle$  with the corresponding Bogoliubov-transformation matrices  $U' = Ue^{i\phi}$  and  $V' = Ve^{-i\phi}$ . We set  $\phi = \pi/10$  and for convenience, we randomly generate the unitary matrices  $D$  and  $C$ . We calculate  $\mathcal{O}^{\text{PN}}$  with Eq. (11) for different values of the number  $n$  of canonical basis states including in the computation [we label  $\mathcal{O}^{\text{PN}}(n)$  the values obtained when  $n$  states are included]. The exact value is obtained for  $n = N = 1938$ , i.e., when all single particle states have been included. Results of the calculation are shown in Fig. (1). Panel (a) shows the modulus of the matrix elements as a function of  $n$  and as one can see, the value of the matrix elements smoothly converges to the exact value as  $n$  is increased. Panel (b) shows the modulus of the real and imaginary part of the relative error defined as  $\delta(n) = [|\mathcal{O}^{\text{PN}}(n) - \mathcal{O}^{\text{PN}}(N)|]/|\mathcal{O}^{\text{PN}}(N)|$ . In order to have a relative error less than one percent around 800 states are needed. Panel (c) shows the decimal logarithm of  $\prod_{i,i'}^n v_i v_{i'}$ , i.e., the denominator of the prefactor of Eq. (1) as a function of  $n$ . The horizontal dashed line and arrow indicate the value  $10^{-322}$ , below which the computation of the overlap with Eq. (1) is numerically unstable when computed with the double-precision data type. In such a case, the computation limit is reached at  $n = 323$  for which  $v_i = 0.097593$ . Increasing the numerical precision would allow us to extend the range of validity of using Eq. (1) to compute the overlap albeit at the price of a higher computational burden. Since in the general case the product  $\prod_{i,i'}^n v_i v_{i'}$  may become arbitrary small, any calculation of Eq. (1) with increased precision will eventually fail.

With the new formula all states can be included without encountering any numerical instability. The ability to include all states is expected to be particularly important for the description of the radial tail of the wave function. A correct description of the wave function at large distances is in turn critical for many applications involving scattering and reaction processes [34] such as alpha decay [35] or the computation of nucleon-nucleus optical potential [36–38].

*Conclusion.*—In this Letter we have presented a new, exact, and numerically stable formulation of overlap

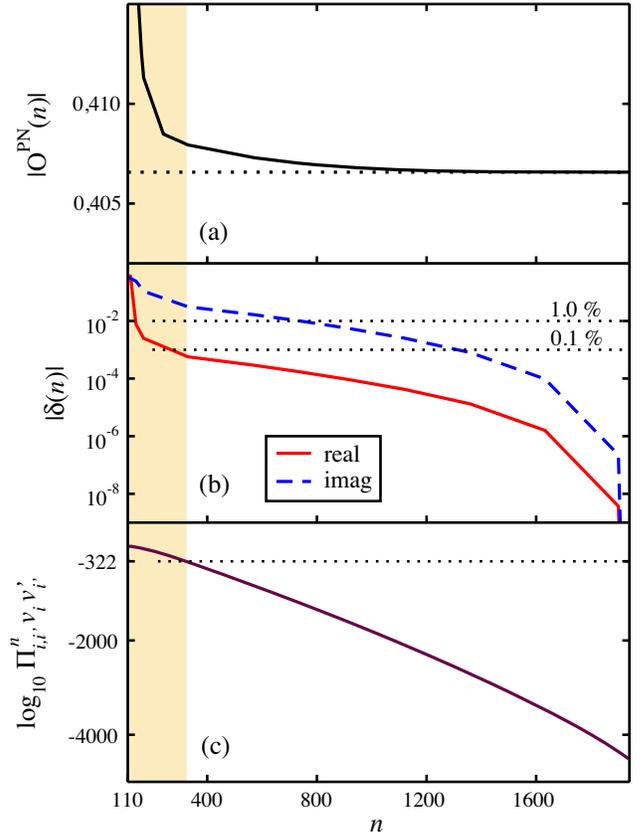


FIG. 1. Matrix element  $\mathcal{O}^{\text{PN}}(n)$  as a function of the number of canonical basis states included in the computation  $n$ . Panel (a) shows the modulus of the matrix elements at  $\phi = \pi/10$  as a function of  $n$ . The dotted line corresponds to the value in the full model space when  $n = N$ . Panel (b) shows the absolute value of the relative error  $\delta(n)$  for both the real part (full line) and imaginary part (dashed line) of the matrix element (see text). The two horizontal dotted lines indicate the error at 1% and 0.1%. Panel (c) shows the decimal logarithm of the denominator of the prefactor in Eq. (1). The horizontal dotted line indicates the value  $10^{-322}$ , which corresponds approximately to the smallest number that can be represented using the double-precision data type. The shaded area represents the range of validity of using Eq. (1) to compute the overlap at the double-precision level.

functions that appear in beyond mean-field theories such as the GCM method. We have illustrated the benefits offered by this formulation by computing a matrix element for the particle-number projection method. We want to emphasize that the derivations presented here are applicable to overlap functions in the context of both even and odd number parity.

The expression for the overlap can be combined with approaches to obtain the matrix elements of the Hamiltonian for example by expressing these matrix elements in a factorized form as sums of products of transition densities multiplied by overlap functions [5,39]. Such transition densities are efficiently calculated in the canonical basis where dimensions can be reduced by

removing unoccupied states [40–44]. The expressions derived in this Letter may also be extended to cover cases when the left and right vacua are expressed in different bases (see, e.g., [22,27]).

The new formula offers substantial improvements over current methods since exact values can now be obtained even in large spaces without being limited by the ability of representing very small or large numbers. It adds no extra computational effort or complexity and may be truncated in a systematic way, which allows for a smooth convergence toward the exact value. Finally, the new formula opens the door toward precision calculations of nuclear reactions and nuclear structure where one takes advantage of the power of symmetry breaking.

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